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Verification and Validation Plan for the Codes LSP and ICARUS (PEGASUS)

**Merle E. Riley, Richard Buss, Robert Campbell,
Matthew Hopkins, Paul Miller, Anne Moats, William Wampler**

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

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Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185-0836

Abstract

This report documents the strategies for verification and validation of the codes LSP and ICARUS used for simulating the operation of the neutron tubes used in all modern nuclear weapons. The codes will be used to assist in the design of next generation neutron generators and help resolve manufacturing issues for current and future production of neutron devices. Customers for the software are identified, tube phenomena are identified and ranked, software quality strategies are given, and the validation plan is set forth.

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Verification and Validation Plan for the Codes LSP and ICARUS (PEGASUS)

I. Introduction

PEGASUS is a name that is used to encompass the ASCI codes which are being used to simulate the operation of the neutron tube. LSP and ICARUS are the two independent ASCI codes being developed to accomplish the simulations. Details of these and other non-ASCI components to the simulation are described below.

The neutron generator, with its neutron tube (NT) component, is one of Sandia's birthright responsibilities in the nuclear weapons program, being part of the "arming, fusing, and firing" directive for Sandia. The suspension of all full-scale testing of nuclear weapons gave impetus to the ASCI (Accelerated Strategic Computing Initiative) campaign of the Department of Energy in the Stockpile Stewardship Program¹. ASCI puts forth the vision that computer simulation can be brought to the point of credibility such that full-scale testing is not necessary for certification of the stockpile or for the design of new weapons. It should be noted that the national weapons laboratories are doing experimental R&D on sub-critical aspects of weapons – there is no reason to expect simulations to be the only resource for most of our work. One has only to consider the major existing and proposed activities in the budget, NIF at LLNL, DARHT at LANL, and MESA at SNL, to see that ASCI is not expected to proceed alone. It would be a misunderstanding of the ASCI effort to assume that certification of weapon systems can be achieved without any experimentation.

The end goal of the ASCI program is to aid in the replacement of full-scale testing, but a penultimate benefit is to economize on the maintenance of the stockpile and the design of new weapons and parts. This activity in weapon design must continue because technology and science are changing rapidly. For example, vacuum tubes have been replaced with solid state electronics, safing mechanisms must be upgraded for new threats, and so on, ad infinitum. Thus both stockpile maintenance and design are to be kept in mind as drivers for the simulation codes that are the product of this investigation.

The codes being investigated in this V&V (verification and validation) plan are for simulation of the plasma-containing part of the neutron generator, the neutron tube. The plasma in the NT includes regions of both high and low density, making the global simulation difficult. A cartoon picture of newer design tubes is included in Appendix B. A physics-oriented description of the tube and its function is as follows: A high voltage from the electrical supply is applied across electrodes in the source region, creating a trigger discharge which evolves into a major discharge or arc, releasing hydrogen plasma within the source region. This plasma is of high density (in the plasma physics' sense) and expands outwards in a plume to enter another higher voltage acceleration region. There the hydrogen ions are accelerated to a target electrode. A metallic screen in the newer design tubes (also called the grid) is used to fix the point of transition (Bohm point) between the expansion region and the acceleration region (called the optics region in Appendix B). Within the acceleration region the plasma is of low density and mostly ions. From this description, a person knowledgeable in plasma simulation can see the

major difficulties inherent in accurately describing the whole process, especially in full dimensionality and geometric detail: (1) We need a time-and-space-dependent simulation of the growth of the plasma from breakdown to full current and expansion. (2) The discharge may have magnetic effects and electrode “spot” behavior. (3) The solution must contain a transition through the Bohm point and describe both the high and low-density regions. (4) The acceleration region can contain effects of space charge and secondary impact processes.

It is necessary to have a perspective of a computer simulation of such plasmas. Although the physical sizes are quite different, a comparison to the simulations of the plasmas involved in magnetic confinement fusion comes to mind since the atomic species are similar. One can easily estimate that more than 10000 man-years of work have gone into simulation and theory of controlled fusion. The simulations there, as here, require numerical analysis, atomic data on hydrogenic systems, massive computational resources, models of complex physical phenomena, and “computer artistry” to complete. To date, despite the fact that important insights have been gained from use of the codes developed in the fusion program, no one would claim that the magnetic fusion simulation tools are predictive at the level of accuracy needed to design a fusion reactor independent of experimentation.

The vision of this effort is to produce codes that can simulate the NT plasma with enough credibility that many of the design and performance issues can be evaluated via computation when used by expert operators. It is necessary that the V&V plans include descriptions of qualified operators and analysts.

Ownership of this V&V plan is assigned to Richard Griffith, manager of the plasma, aerosol, & noncontinuum processes department, in order to assure stability in the oversight of V&V progress. V&V coordination is delegated by him to individuals active in the V&V implementation, currently Anne Moats for the DSMC activities and Merle Riley for the LSP simulations. It is the responsibility of these three individuals to review periodically the V&V plan to ensure that it remains current and useful. This V&V plan was developed through the collaboration of a large number of experts. The PIRT chart from the original version of this plan is being included as an appendix (Appendix B) because it was never published and this serves to preserve the plan for future reference. These plans were constructed by extensive discussions between the code development teams (including Richard Griffith, Justine Johannes, Timothy Bartel, Seung Choi, Michael Gallis, Thomas Otahal, Anne Moats, Richard Buss, Tom Mehlhorn, Barry Marder, Dale Welch, Merle Riley, Robert Campbell, Tim Pointon, Becky Coats, Mark Kiefer), the NT design and manufacturing people (including, Bud Burns, Robert Koss, Gary Laughlin, Carla Busick, Frank Bacon and John Brainard) and the experimentalists funded by MAVEN (Paul Miller, Greg Hebner, Bill Wampler, Don Cowgil). For several years, there have been biweekly meetings of the neutron tube modeling effort with broad participation by the various teams to discuss developments and exchange information. This current version of the V&V plan is the result of extensive rework of the original plan by the primary author with input from the teams.

Note that a revised version of this plan will be prepared next year in response to feedback from the V&V Peer Review Process.

II. Stockpile Drivers and Customers

The Stockpile driver for this ASCI work is the performance of the MC4300 and MC4277 neutron tubes when operated using the standard source and target materials, and operated using a normal range of power supply output. The tube performance includes many characteristics such as time to arc initiation, beam current to the target, and beam spatial profile on the target. There are many drivers of more limited scope. An example is the effect of helium pressure on the tube performance and lifetime. It is our opinion, developed through many discussions with the tube design and tube manufacturing groups, that these other drivers are subordinate, and necessitate accomplishment of the main driver as a prerequisite. The effect of helium cannot be evaluated unless the codes can successfully model the performance of the tube under standard conditions. The NT simulation codes must be able to calculate accurately the performance of existing designs in the stockpile. Moreover, due to the necessity of continuing new design, it is expected that the simulation codes will be robust enough that they can predict the scaling and performance changes of any new designs of the NT. The two major customers are the neutron tube design groups associated with any replacement parts or new designs and the neutron generator manufacturing organization. The tube design group needs code which can address issues such as the optimum geometry for achieving adequate ion beam quality. The tube manufacturing team requires a code which can evaluate the effects of part tolerances on tube performance. The product of this activity is a code or suite of codes that can simulate the NT from the input electrical signals to the output of neutrons with qualified operators.

III. The Code Inventory Applicable to the NT Plasma

Due to the sore lack of existing codes capable of simulating the NT plasma at a fundamental level, some code development is necessary in order to adapt existing codes to the problem. Thus we must describe the starting point for the V&V process on these codes.

One of the first codes applied to the NT is SPC (Simple Plasma Code) of Barry Marder² at Sandia. The earliest version of this code³ was developed in 1977 in the NT program at Sandia. This steady-state code is 2-D (two-dimensional) and solves the plasma with the following assumptions: (1) a Boltzmann electron approximation, (2) non-iterative numerical solution of the Poisson equation, and (3) an ensemble of ion trajectories for the ion density. With many features and restrictions that we will not describe here, the code can simulate the expansion from a surface outside the high-density arc to the screen transition region, through the screen, and solve for the ion motion in the high acceleration region. This code runs fast and is useful for simulations of restricted regions of the NT plasma. However it is not easily converted to 3-D (three dimensions), is not time-dependent, and is probably not useful in the high-density arc region where the geometry is inherently 3-D.

The commercial code PC-Opera has become a mainstay of the NT design effort at Sandia over the last five years. This code is not a plasma code so much as a Poisson solver with very flexible geometry and spatial gridding. The code is steady-state and 2-D, with 3-D versions now available. PC-Opera has the ability to do independent-ion trajectories within the field that it calculates. Thus it is very useful for most design issues

related to the high-field acceleration region of the NT. It is not capable of doing the high-density region or the expansion to the screen, or the screen region itself except as an input boundary condition. This code is fairly easy to set up with geometric input and runs fast on a personal computer platform.

The Sandia code ICARUS⁴ based on the DSMC (Direct Simulation Monte Carlo) method for simulation of rarefied gas dynamics and chemistry is available. In this report we use DSMC to refer to all versions of the original code that have been modified to solve for plasma electric fields. This Fortran code has undergone much development by Tim Bartel and coworkers as to MPP (massive parallel processing), benchmarking with neutral gas flow and chemistry, and flexibility of geometry. The code is designed with a flexible “patchwork” spatial grid, which is ideal for a problem not requiring the solution of field equations. The particle solution mechanics within the code are similar to those within a PIC plasma code, but the lack of a numerical gridding scheme compatible with the Poisson equation causes difficulties. The code is also not implicit in the time evolution, which restricts the practical applications to the regions of lower plasma density. The regions of low density in the present NT designs are 2-D in symmetry, which is compatible with the 2-D nature of the most developed version of the DSMC code.

Sandia is currently using under license the plasma code LSP (Large Scale Plasma)⁵, which is an evolving product of Mission Research Corporation. Earlier versions of LSP were in use in the code IPROP. LSP was designed from the ground up to be a 1-D, 2-D, or 3-D plasma code with implicit time evolution, moderately flexible geometry and chemistry, and running in MPP. The code suffers from not having a responsible Sandia division or person, and from being somewhat tedious to set up with input files and controls. This proprietary code is written in C, and runs on most of the MPP (massive parallel processing) environments at Sandia. Current features under development by MRC include magnetic fields and MPP enhancements⁶. LSP alone is capable of 3-D simulations which are required in the high plasma density source region of the NT.

Another possibility for simulation of the NT was to obtain a plasma code from the “outside,” either from a university or other laboratory. This would involve a tremendous amount of learning, analysis, benchmarking, and development of the code. This is the same amount of work as developing a new code for the NT simulation. It is believed that the best choices are from among the codes mentioned above. The two smaller codes, PC-Opera and SPC, are to be used for localized problems within the overall NT simulation and will not be entered into the V&V process. The two larger codes, ICARUS and LSP, have been subjected to additional development, and are in the V&V process for application in the ASCI program. This V&V plan for LSP and ICARUS is based loosely on the guidelines developed by Pilch et al⁷. Codes in the process of development that may reach productivity in the time scale of five or more years are not addressed here.

ICARUS, the DSMC code, is currently a choice for solving the NT plasma from outside the high density region “onwards” to the target. DSMC has proven itself capable of high-fidelity meshing of the geometry and structures. The symmetry of the NT is cylindrical in this region, which is compatible with DSMC. Unfortunately the high-density region remains a difficult problem for DSMC. Currently when we desire an end-to-end simulation of the NT plasma, the plan is to use the output of LSP for the source

region as input for DSMC. Currently DSMC operates by dividing the computational zone into an ambipolar region and a full-field-solve zone that utilizes the Poisson solver. This requires a matching procedure between these zones, an algorithm which is still being developed and verified. In the acceleration region of the NT, DSMC needs to incorporate the dielectrics into the Poisson solver. This development will result in a DSMC code that is capable of major improvements on the PC-Opera code now in use for the acceleration region. DSMC is quite flexible for geometry input and chemistry⁸.

The LSP code has proven that it can solve a two-electrode model of the 3-D high-density region of the NT with good success. LSP has also shown that it can carry out a 2-D simulation of the whole NT including a limited model of the source, the expansion region, the screen, and the optics region. What remains to be done is to prove that the transition of the initial breakdown from the trigger T-K to the A-K discharge can be done with a reasonable spatial grid and computation time. Improvements need to be made on the kinetic mechanisms for electron and ion impact on the surfaces, including the material hydrogen release model. These mechanisms are crucial for predicting the delay and rise times for firing of the NT. One problem is the long computation time required for these simulations. The turn-around time for a 3-D run is of the order of a week or more on any of the MPP machines. Some work needs to be done to quantify MPP efficiency as relates to spatial grid resolution needed to describe the geometry of the NT. It is understood that the trigger mechanism itself will be allocated to a “sub-grid” model and not required in the simulations. The time involved in the trigger is negligible compared to the transfer of the discharge from the trigger to the full source current.

MAVEN experiments have been extremely helpful in code development and validation⁹⁻¹¹. Probably only in-house experiments are worth doing, unless some specific cross section or rate or property can be done quicker on the outside. MAVEN contributions include the following: (1) Quantified the material hydrogenic release rates. (2) Showed the nature of the T-K to A-K transfer in the trigger mechanism. (3) Suggested surface mechanisms (or lack thereof). (4) Given visual pictures of species in the discharge, including Scandium. (5) Measured the spatial properties of the expansion plume. (6) Given graphic evidence of evolving material structure on the electrodes. The future MAVEN plans, even if not connected to a specific validation run of the codes, will be a valuable asset to the understanding of the NT operation. MAVEN can be useful in supplying unknown or incalculable quantities that enter the simulations.

IV. The PIRT (Phenomena Identification and Ranking Table)

Through extensive meetings and discussions between the code development teams, the tube design team, the tube manufacturing team and experimentalists working on the tube physics, a list of the phenomena associated with the tube performance was assembled. This list was incorporated into the PIRT in the earlier version of the V&V plan (Appendix B). Further refinement of this list has resulted in the following PIRT, Table 1.

This PIRT is divided into sections that relate to different physical regions of the NT. The first section is the source (S) region containing the trigger and other active electrodes. The second section is the plasma expansion region, sometimes referred to as the plasma cup (C). The third section of the table is the screen region, referred to as the grid (G) in the prior PIRT plan. The fourth section of the table concerns the high-field acceleration region of the NT, called the ion optics (O) region.

The first column in the PIRT contains the physical phenomena requiring simulation. The second column briefly describes the activity necessary to verify and/or validate a particular code. All items are marked with a literal description. Importance is labeled as “major,” “moderate,” “minor,” or occasionally “unknown.” The adequacy of the simulation is labeled with “good,” “fair,” “poor,” or “unknown.” Such labeling is not a comment on the existing software, but what is known about the use and validation. It is not felt that a further subdivision of this ranking is warranted.

Phenomena	Description of activity needed to complete the V&V process	Importance to success	Adequacy
Source (S) region			
(1) Hydrogen release from Scandium hydride storage material.	Activate material model for release of hydrogen due to arc heating in LSP code. Validate against MAVEN data.	major	good
(2) Transfer of discharge from T-K gap to the A-K gap.	In LSP, improve the electron and ion surface process description. Verify with literature if available. Validate against MAVEN data.	moderate	poor
(3) Delay and rise times of source current and plasma production.	Validate LSP against MAVEN and other available data.	major	fair
(4) Release of non-hydrogenic ions from the source and trigger.	MAVEN experiments must try to quantify release conditions and rate, material model must be developed.	moderate	poor
(5) Non-uniform radial heating of electrode.	Validate LSP predictions of deposited energy with MAVEN data.	moderate	unknown
(6) Structural and chemical changes in hydrogen storage medium.	The physics of this must be resolved into a “sub-grid” description in the material model incorporated in LSP.	unknown	poor
Expansion cup (C) region			
(1) Electron and ion temperatures and ion energy.	LSP and DSMC need validation against MAVEN data. DSMC needs verification of electron algorithm	moderate	fair

(2) Flow of plasma around throttle plates and obstructions.	LSP and DSMC need to be validated against MAVEN data .	major	unknown
(3) Free expansion of high-density plasma in arc to lower density near the screen.	LSP and DSMC must both solve this region to verify codes and transfer information. Validate against extant MAVEN data.	major	fair
(4) Magnetic self-field effects on plasma expansion and arc.	Magnetic fields are to be tested in LSP.	unknown	fair
Screen or grid (G) region			
(1) Plasma penetration through screen.	Need study of plasma “meniscus” in vicinity of screen for all codes. Test cell resolution in LSP.	major	fair
(2) Ion deflection by screen and space charge. Variation of current with geometry.	Need comparison to data and SPC code for ion ballistics at and beyond screen for both LSP and DSMC.	major	fair
(3) Expansion-to-acceleration transition for designs without material screen.	LSP and DSMC need verification that free Bohm point can be simulated.	moderate	poor
Acceleration optics (O) region			
(1) Electric field in acceleration region.	Verification needed for the treatment of dielectrics in DSMC Poisson solver using analytic models.	moderate	good
(2) Precision of ion optics and tolerances.	DSMC needs to be developed in 3-D in order to assess these defects.	minor	poor
(3) Scattering within acceleration region, production of secondary electrons within region.	Kinetic data needed in DSMC and LSP for released neutral gas.	major	poor
(4) “Gassing” with age of NT, primarily in optics region.	Codes must be able to assess effects of aging on performance.	moderate	poor
(5) Charging and secondary electron processes on the dielectric materials in acceleration region.	Verification and validation needed against literature or MAVEN data for LSP and DSMC.	major	fair
Integral (I) or global phenomena			
(1) Shot lifetime for multiple test firing of NT.	Validation needed for comparison to data on shot lifetimes.	major	fair
(2) Latency effect in full NT operation for multiple firings.	Need MAVEN investigations and probably additional surface kinetics.	major	poor
(3) Full NT operation.	Resolve MPP efficiency of LSP for 3-D problems as to domains, processors, grid decomposition	moderate	fair
(4) Full NT operation.	Better code transfer of information from LSP to DSMC.	moderate	fair
(5) Full NT operation.	Resolve computer hardware issues concerning availability of MPP machines for long LSP and DSMC runs.	major	fair

TABLE 1. PIRT chart

We note that the form of the previous PIRT has been simplified in two ways. First, there is not much reason to separate out neutron production and design scaling; both require much the same advances and testing. Second, we include a short description of the code improvements or activity necessary to address the phenomena in the PIRT list. This avoids the necessity of constructing a second table of code developments that must be cross-correlated with the PIRT.

V. Software Quality Engineering

Icarus uses MERANT PVCS Dimensions 6.0 for source control. Dimensions imposes a formal system tailored to meet the DSMC team requirements to control code modification. The structure of code management for Icarus was determined through a series of meetings of the DSMC team with representatives from Merant. Icarus and its utilities reside in the Dimensions repository. Software change requests are formally entered, approved or rejected following DSMC team discussion, implemented and reviewed. This system of code control may be too elaborate and costly for such a small code development team, but ICARUS is being used to test implementation of this professional code management system, in anticipation that it may be used for other ASCII codes such as SIERRA in the future.

The DSMC team has biweekly meetings, independent of the biweekly neutron tube modeling meetings, in which the software change requests are discussed and acted upon. Questions of software engineering standards are often discussed, and it has been agreed that ICARUS will require significant work to improve documentation. The current user's manual is woefully inadequate and a plan is in place to upgrade the manual interactively using the Dimensions framework.

LSP uses CVS (Concurrent Versions System) to maintain revision control. CVS provides revision control for a collection of LSP files. These files are combined together to form a software release. CVS provides the functions necessary to manage these software releases and to control the concurrent editing of source files among multiple software developers. CVS keeps a single copy of the LSP source. This copy is called the source "repository;" it contains all the information to permit extracting previous software releases at any time based on either a symbolic revision tag or a date in the past. Three copies of the repository, on different machines, are kept and updated every day.

VI. Verification Test Suite

The existing set of test problems for verification of ICARUS were not derived directly from consideration of the PIRT for this V&V activity. ICARUS has been under code development (principally by Bartel) for over ten years. A set of verification tests have been constructed to check that components of the code are correctly implemented. The pertinence of various test problems to the neutron tube calculations varies considerably, but at this stage of code development, all tests are used to evaluate the code performance. A test which verifies the correct energy exchange between diatomic species is not currently deemed useful for tube modeling. The DSMC team plans to derive a more

restricted set of test problems ranked for importance to the specific tube simulation, but at present uses a higher standard, that the code must pass all verification tests.

We have compiled a body of test problems, summarized in Table 2, to either test ICARUS results for correctness (verification) or to insure code changes do not introduce unexpected changes (regression testing). Some of the following problems have an exact numerical answer that can be compared with standard regression testing methods. However, there is a class of solutions that are stochastic in nature that require a more complex method of verification. A code has been written to compare stochastic solutions based on statistical analysis of the variation from a sample of solutions. That effort is still underway. The ultimate goal is automated regression testing of ICARUS and its utilities.

In Table 2 an attempt has been made to estimate code coverage of the tests. These estimates are very crude at present. The question of how much of the code is tested is difficult to estimate at best, whether lines of code exercised, % of relevant code or whatever. We are exploring available software for quantifying code coverage and best practices for assuring adequacy of testing. Note that the % coverage figures in the table are highly overlapping and do not allow one, as yet, to answer the question- how much of the code is verified.

Test Name	Description	Area of Code Tested
Grid tests	A suite of geometrical meshing problems, including curved surfaces, shape functions, grading of gridlines	Tests approximately 60% of the meshing utility Init2d
Chemically reacting flow over a wedge	Chemically reacting flow of air over a wedge.	Collisions, energy exchange, chemistry. (~20% of code)
Box decomposition	Tests the static domain decomposition of the Poisson solver. Also tests parallelization issues.	Tests 50% of the Poisson solver portion of ICARUS
Cc test	Constant volume charge test used to ensure the Poisson solver is considering volume charge correctly in both Cartesian and cylindrical coordinates.	Tests 70% of the Poisson solver.
Dielectric H sheath	Tests the dielectric material modeling as well as surface charging.	Tests 95% of the Poisson solver. This solution is stochastic.
Sphere	Sphere with electrostatic boundary conditions. Tests the accuracy of the Poisson solver on non-linear geometries and axisymmetric boundary-element-method.	Tests 60% of the Poisson solver.
Child-Langmuir box	Ion and electron source flowing across a region, limited by Child-Langmuir current limits.	Tests space-charge effects of the Poisson solver – 20 % of the Poisson solver.
Free Expansion	Expansion of a plasma into free vacuum. An analytic solution for spatial distribution and molecular velocities.	Tests moves, collisions, chemistry, ambipolar to full-field transition. This is a stochastic solution that tests 50% of the code overall.
Simple screen	A simple grounded grid with particles streaming through.	Tests the Poisson solver, ambipolar to full-field transition, and particle transport. A stochastic solution that tests 30%.
Neutron generator (classified)	A typical neutron generator tube geometry with typical current/voltage characteristics	A global tests of most areas of the ICARUS code. A stochastic solution that tests 70% of the entire code.

TABLE 2. Current Test Suite for ICARUS

MRC tests the LSP code using a large number of test problems¹³. In addition, for the tube arc simulations, the following three test problems are used for verification. These problems do not have exact numerical solutions.

- 1) End-to-end 2-D source to target tests 98% of relevant coding (it tests 100% of relevant physics, not all of the geometry).
- 2) 2-D "source only" simulation tests 95% of relevant coding.
- 3) The 3-D arc "source only" tests 95% of relevant coding.

VII. Validation Plan

As the major activities concern the two available codes, DSMC and LSP, we present the major work activities necessary to bring the codes through the validation process. This discussion *combines* a milestone chart with code modifications as was presented in Sections 4 and 5 of the former V&V plan. No labor or timetable is assigned to this activity, since the available funding and manpower is uncertain at the time of writing. A detailed plan of work must be cross-correlated with this V&V plan, even if only informally. The items are listed in a suggested *order of activity* however. In addition to the DSMC and LSP activities, we include a list of MAVEN experiments which would be very valuable for the V&V objectives. Not all of these experiments may be realizable in practice, and they are not ordered in importance or time. A tentative FY02 Milestone Chart is included in Appendix A. In the list below, the corresponding item in the PIRT chart is given, i.e. S1 is the first item under Source in the PIRT chart. Essentially all items in the PIRT chart are included in the plan except for several items such as G3 and O2 which are much longer term and dependent on future funding resources.

A. DSMC Activities:

- (1) The particle move algorithms must be “debugged” to handle the implementation of curvilinear cell walls. This is underway. (C3, G1, I1)
- (2) Dielectric media and charge accumulation on surfaces have been incorporated into DSMC but these features have not yet been validated. (O1, O5)
- (3) The transition in the plasma expansion region (“cup”) from the ambipolar approximation to the full-field-solve equations must be formalized from plasma theory and implemented in the coding. (C3, G1)
- (4) The kinetics for He neutral gas interacting with the other plasma species must be included. Inclusion of helium may require some code modifications to allow for differential species weighting. (O3, O4, I1)
- (5) The input of data to DSMC from the output of LSP solutions of the source region must be tested and possibly refined. (I4)
- (6) DSMC and LSP solutions will be developed and compared from the pre-screen (expansion) region to the target. This will be a major benchmark for the simulations that includes all regions of the NT outside the source arc region.
- (7) Validation of flow around obstacle (existing MAVEN data). (C2)
- (8) Continue comparisons of full tube calculations MC4300 and MC4277. (G2)

B. LSP Activities:

- (1) Initiation of the source arc including the transfer of the discharge from the trigger to the main arc discharge. This will be done in 3-D with the full three-electrode model of the source. (S2, S3)
- (2) An input file for LSP will be developed for the screen and acceleration regions. LSP solutions can then be compared to DSMC from the pre-screen (expansion) region to the target. This will establish a benchmark between the codes as well as prove the global capability of LSP to simulate the whole NT.
- (3) Activate the material release model for the active electrodes. Validate heating of electrodes against known data. Necessitates secure platform for computations. (S1, S5)
- (4) Self-consistent magnetic field algorithms in LSP will be used to compare to available MAVEN results. (C4)
- (5) The output of LSP in the expansion region will be studied as to the best manner of transferring information to DSMC. (I4)
- (6) Resolve MPP efficiency of LSP as to number of domains, processors, and grid decomposition necessary for simulation of whole NT. (I3, I5)
- (7) LSP particle algorithms are to be incorporated into the ALEGRA framework in order to achieve a robust platform in the context of Sandia's code maintenance.

C. Experimental Activities:

Note: This is a list of experimental measurements which are highly desirable for validating these codes.

- (1) Diagnostics of trigger-to-main arc transition on a fast time scale to elucidate the firing mechanism of the ion source. This will require framing camera operation. The results will aid in the validation of LSP simulation of the delay, rise-time, and mechanism of breakdown. (S2, S3)
- (2) Study of trigger-to-main arc transition with and without non-refractory materials present in order to test the importance of ion release from the electrodes. (S2, S4)
- (3) Time resolved ion energy measurements in the expansion region ("C") above the source, needed to provide additional insight into the mechanism for ion energy gain in the expansion and validation of the LSP simulations in this region. (C1, C3)
- (4) Testing of ion sources using different hydrogen storage materials to find if refractory metals other than Scandium are advantageous. This may require development of a new hydrogen emission model for the storage material. (S1, S6)

(5) Infrared (IR), thermal imaging of storage material subjected to repeated firing to ascertain uniformity of heating and material changes. (S5, S6)

(6) Measurement of secondary particle production due to ion and electron impact on surfaces. This can include relatively high energy ions in the target area as well as the lower energy electron and ion impacts in the growth of the main source arc. (O1, O5)

(7) Study of varying geometry (electrode spacing, orientation, shields, throttles, etc) to improve design and to support validation of the codes.

VIII. Stockpile Computing

Lee¹² has pointed out the need to designate appropriate guidelines for doing stockpile calculations. However, guidelines for use of computational tools in the design, manufacture and certification of stockpile components are still under development. An example of the needed guidelines is that test problems must be run on the specific computing platform that will be used for the stockpile computations. This recognizes the platform dependence of code verification. It is also essential that the code V&V encompasses the parameter space needed by the stockpile application.

Documentation in reproducible detail is essential for the entire simulation process for each stockpile calculation. This must include at least such detail as the computing platform and operating system, the compiler, the version of the code, and all the input parameters and gridding detail which are used. The documentation must be sufficiently complete that the precise calculation can be reproduced at a future date if required.

As currently implemented, ICARUS requires an expert user with extensive hands-on experience in order to obtain a single useful calculation. The input structure is extraordinarily complex and ill-documented. Much current activity by the DSMC team is associated with moving the code toward production quality such that the level of training necessary to achieve stockpile computing competency will be reasonable.

LSP is similar in the level of expertise needed. A great deal of training and experience is currently required to achieve a correct arc simulation.

Currently, a single end-to-end simulation of the neutron tube operation using ICARUS is achieved on the Intel teraflop platform using 500 processors for 24 hours. A 3-D simulation of the arc with LSP may require many weeks on 50 processors. Code improvements and hardware advances are expected to bring these times down, but at this time stockpile computation with these tools is quite computer-resource intensive.

It should be noted that more detailed and comprehensive stockpile computing guidance is being prepared by the ASCI program to support all of the code projects, and that this material will be incorporated when it becomes available.

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IX. APPENDIX A

FY02 Milestone Chart for the NT V&V Plan

1Q FY02:

- 1) Initiation of the source arc using LSP, including the transfer of the discharge from the trigger to the main arc discharge. This will be done in 3-D with the full three-electrode model of the source.
- 2) The particle move algorithms in DSMC will be “debugged” to handle the implementation of curvilinear cell walls.
- 3) Time resolved ion energy measurements in the expansion region (“C”) above the source. Additional insight into the mechanism for ion energy gain in the expansion, and validation of the LSP simulations in this region.
- 4) Infrared (IR), thermal imaging of storage material subject to repeated firing to ascertain uniformity of heating and material changes.

2Q FY02:

- 1) Self-consistent magnetic field algorithms in LSP will be used to compare to available MAVEN results.
- 2) An input file for LSP based on a model source geometry and physics will be developed for the source, screen, and acceleration regions. The success of this simulation will prove the capability of LSP to simulate the whole NT.
- 3) Dielectric media and charge accumulation on surfaces will be incorporated into DSMC.
- 4) In DSMC, the transition in the plasma expansion region (“cup”) from the ambipolar approximation to the full-field-solve equations must be formalized from plasma theory and implemented in the coding.
- 5) Diagnostics of trigger-to-main arc transition on a fast time scale to elucidate the firing mechanism of the ion source. This will require framing camera operation. The results will aid in the validation of LSP simulation of the delay, rise-time, and mechanism of breakdown.

3Q FY02:

- 1) The kinetics for He neutral gas interacting with the other plasma species must be included in simulations. Inclusion of helium may require some code modifications to allow for differential species weighting.
- 2) Testing of ion sources using different hydrogen storage materials to find if refractory metals other than Scandium are advantageous. This may require development of new hydrogen emission model for storage material.
- 3) LSP will carry out validation simulations to compare to the MAVEN data on main source arc delay and rise of current. Validation of firing mechanism.
- 4) LSP will initiate tests of storage material execution on a secure platform.

4Q FY02:

- 1) The input of data to DSMC from the output of LSP solutions of the source region must be tested and possibly refined.
- 2) DSMC and LSP solutions will be developed and compared from the pre-screen (expansion) region to the target. This will be a major benchmark for the simulations that includes all regions of the NT outside the source arc region.
- 3) LSP particle algorithms are to be incorporated into the ALEGRA framework in order to achieve a robust platform in the context of Sandia's code maintenance.

X. APPENDIX B

1999 Neutron Generator Modeling and Simulation Validation Plan

Introduction:

Simulation of the Neutron Tube (NT) has been divided into the following four areas: source discharge, plasma cup, grid, and optics. Separating the tube into different simulation regions was required due to governing local physics, and simulation length scales. Figure 1 is a sketch that defines the four regions. Each region will require a separate validation plan. However, results from one region will define the boundary conditions for the next region, requiring a tight coupling of the simulations. Simulations will be required to predict transient tube performance as a function of: source power, tube pressure, surface conditioning/material, and shot number. The PIRT chart will rank the importance of the phenomena and the status of the model development/understanding.

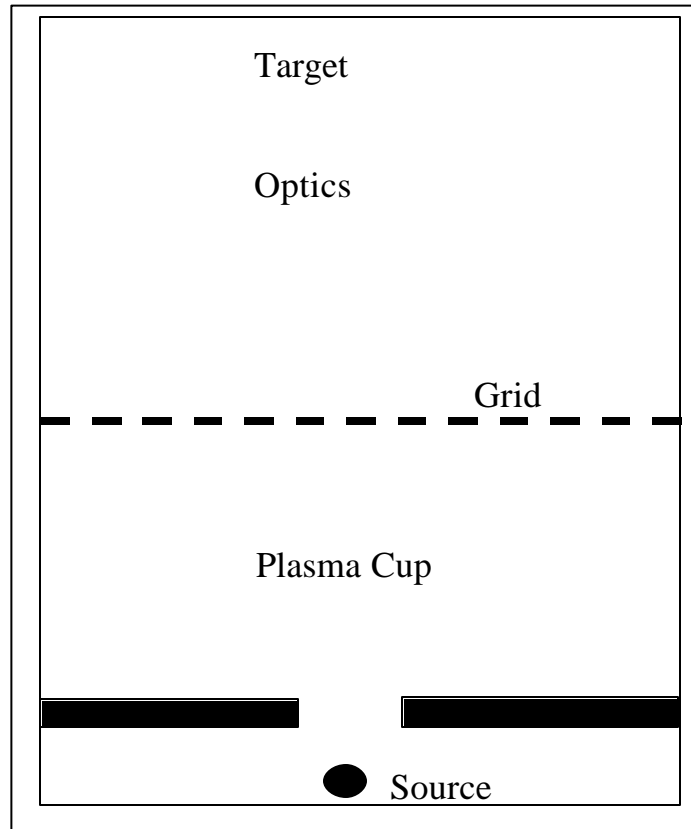


Figure 1. Generic Neutron Tube Region Definitions

Phenomena Identification and Ranking Table (PIRT)

This section will give a bottom-up review of the phenomenological models in the NT simulation codes. The impact of the models in predicting NT performance will be ranked along with the current status of the model.

Neutron Tube Simulation	Importance to Neutron Tube Performance		Adequacy
	Predict Neutron Production	Trends with Design Changes	
SOURCE (S)			
S-1. Power coupling	High	High	Inadequate
S-2 Electrode Conduction Heat Transfer	Medium	Medium	Inadequate
S-3 D ₂ /Sc Desorption	High	High	Inadequate
S-4 D ₂ Source Diffusion	Low	Low	Inadequate
S-5 Surface Effects:			
a. Ion Neutralization	Medium	Medium	Inadequate
b. Recombination	Low	Low	Adequate
c. Thermal/Angular Reflection	Low	Low	Adequate
d. Secondary Electron Emission	Medium	Medium	Inadequate
e. Surface Charging	Medium	Medium	Adequate
f. Surface Conditioning	High	Medium	Inadequate
g. Surface Cracking	High	Medium	Inadequate
h. Cathode Spot Formation	High	Medium	Inadequate
S-6 Electrode Heat Flux	High	Medium	Adequate
S-7 Neutral, ion, and electron densities, and energy distributions.	High	High	Inadequate
S-8. Gas Phase Reactions:			
a. Electron Impact Reactions	High	High	Adequate
b. Excitation Reactions	High	High	Adequate
c. Coulomb Interactions	Medium	Medium	Adequate
d. Charge Exchange Reactions	High	High	Adequate
S-9. Electric fields	High	High	Inadequate
S-10. Magnetic fields	Low	High	Inadequate (?)
PLASMA CUP (C)			
C-1. Inflow Description	High	High	Inadequate
C-2 Surface Interactions:			
a. Secondary Electron Emission	Low	Medium	Inadequate
b. Neutralization	Medium	Medium	Inadequate
c. Surface Reactions	Low	Low	Inadequate
d. Thermal/Angular Reflection	Low	Low	Inadequate
e. Surface Charging	Medium	Low	Inadequate
C-3. Neutral, ion and electron densities and energy distributions	High	High	Adequate(2-D) Inadequate (3-D)
C-4. Gas Phase Reactions:			
a. Electron Impact	High	High	Adequate
b. Excitation Reactions	High	High	Adequate

c. Coulomb Interactions	Medium	Medium	Adequate
d. Charge Exchange Reactions	Medium	Medium	Adequate
C-5. Electric fields	High	High	Inadequate
C-6. Magnetic fields	Low	High	Inadequate
C-7. Sheath	Low	Low	Inadequate
C-8. Outflow Description	Medium	Medium	Adequate
GRID(G)			
G-1. Inflow	High	High	Inadequate
G-2 Surface Interactions:			
a. Secondary Electron Emission	Low	Low	Inadequate
b. Neutralization	Medium	High	Inadequate
c. Surface Reactions	High	Medium	Inadequate
d. Thermal/Angular Reflections	Medium	Low	Inadequate
e. Surface Charging	Low	Low	Adequate
G-3. Neutral, ion and Electron Densities And Energy Distributions	High	High	Adequate
G-4. Gas Phase Reactions:			
a. Electron Impact	Low	Low	Adequate
b. Excitation Reactions	Low	Low	Adequate
c. Coulomb Interactions	Medium	Medium	Adequate
d. Charge Exchange Reactions	High	High	Adequate
G-5. Electric Fields	High	High	Inadequate
G-6. Magnetic Fields	Low	High	Inadequate
G-7. Outflow	Low	Low	Adequate

OPTICS (O)

O-1. Inflow	High	High	Inadequate
O-2 Surface Interactions:			
a. Secondary Electron Emission	High	High	Inadequate
b. Neutralization	Medium	Medium	Inadequate
c. Surface Reactions	Low	Low	Inadequate
d. Thermal/Angular Reflections	Medium	Medium	Inadequate
e. Surface Charging	Medium	Medium	Adequate
O-3. Neutral, Ion, and Electron Densities and Energy Distributions.	High	High	Adequate
O-4. Gas Phase Reactions:			
a. Electron Impact	Low	Low	Adequate
b. Excitation Reactions	Low	Low	Adequate
c. Coulomb Interactions	Low	Low	Adequate
d. Charge Exchange Reactions	High	High	Adequate
O-5. Electric Fields	High	High	Inadequate
O-6. Magnetic Fields	Low	Low	Inadequate
O-7. Neutron Production	High	High	Inadequate

XI. APPENDIX C

Prior Accomplishments in V&V Activities on the NT Plasma

All in all, the prior accomplishments have gone slowly, with the experiments out-racing the simulations in some cases. Experimental determination of basic quantities such as surface coefficients and plasma species' densities has not been completed, however. The plasma NT V&V process was launched under a handicap compared to some other V&V programs where the basic constitutive physics and engineering data were already in hand, but the results for this plasma study are proceeding well considering the necessity of code modifications and development.

Appendix B of this report contains the PIRT chart from the prior V&V plan for the NT plasma. This plan was only partially utilized during the prior activity. The main reason is that the plan was very detailed, and resources were too limited to follow through on all the implied tasks. Some major V&V items were completed though, and we list them here. We follow each item with cross-reference to the old PIRT plan, denoted by the labeling in place there. For example, the magnetic field phenomenon in the old PIRT contained in Section 3., item S-10 will be denoted (3.S-10). Cross-references denoted by (5.C-4) refer to the Validation/Calibration Milestones in Section 5., item C-4, to verify/validate the kinetic chemistry modules. Not all the items overlap exactly in content, so some of the prior V&V items may not be completed as written.

Verification Items

LSP was successfully tested for accuracy of implicit time integration against an exact model solution where the plasma was expanding by ambipolar diffusion. This was a benchmark test in numerical accuracy motivated by replacement of the IPROP code by the newer LSP code.

DSMC and LSP were both upgraded to use essential parts of the hydrogenic cross sections and rates obtained from the scientific literature assembled by William Morgan of Kinema Research & Software for the project. (3.S-8, 3.C-4, 3.G-4, 3.O-4, 5.C-4)

DSMC was supplied with a 2-D Poisson solver based on the boundary Green's function method to accommodate the patchwork grid structure in space. The solver was found to be inaccurate due to the numerical scheme in the boundary elements and this has been revised and verified to give acceptable numerical accuracy in several model field solutions. (3.C-5, 3.G-5, 3.O-5)

LSP was tested in reduced dimension for its ability to reproduce an electron plasma sheath. This was successful for the "kinetic particle" electron mode, but not in the "fluid particle" electron mode. (a general item in the replacement of IPROP by LSP)

LSP and DSMC were successfully benchmarked against Sandia's Quicksilver code and PC-Opera for accuracy in solving the ion motion and field solution in the acceleration region of the NT. (3.O-3, 3.O-5, 5.O-1)

LSP has had the material hydrogen release model installed and executed. This material release model has been benchmarked against much data taken at Sandia and from the scientific literature. (3.S-2, 3.S-3, 3.S-4, 5.S-3)

Validation Items

DSMC and LSP have both been compared for the expansion of the plasma plume against the MAVEN measurements. (3.C-3, 3.C-8)

LSP's prediction of the electron temperature in the expansion plume (cup region) agrees reasonably with the MAVEN measurements. (3.C-3, 5.C-1, 3.C-7)

The stand-alone coding for the hydrogen material release model has been checked against the MAVEN measurements. (3.S-2, 3.S-3, 3.S-4, 5.S-3)

LSP predicts magnetic confinement effects on the expansion plume of the same order as seen in some preliminary MAVEN measurements. (3.C-6)

LSP solution in 3-D with a two-electrode model for the source region predicts an arc current rise and voltage drop in agreement with the tube data. (3.S-1, 5.S-1)

DSMC predictions of the ion impact on the target electrodes and the retarding electrodes in the acceleration region are in good agreement with the trends seen in experiments. (3.O-3, 3.O-5)

LSP output from the high-density source region was fed into DSMC as input conditions to construct a total simulation of the NT. Preliminary tests only, enabling on-target current to be compared to data. (3.C-1, 3.C-8, 3.G-1)

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